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Quasiperiodic interaction with a metal-insulator transition

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We describe a quantum Hamiltonian in one dimension with a quasiperiodic interaction, giving rise to a metal-insulator transition at high coupling. This model applies to a linear wave propagation in a modulated medium, naturally resulting in potentials with incommensurate periods, as is the case for organic linear conductor chains.

Many physical situations deal with a Schrödinger operator with an almost periodic potential. The first historical example goes back to Peierls[1] and describes the one-band Hamiltonian for a Bloch electron in a magnetic field, in the approximation where the interband contributions can be neglected; see Ref. 2.

More recently, the subject became of interest in the context of the search of organic superconductors. As predicted by Little,[3] it seems theoretically easier to get superconductivity at high temperature, using organic material rather than metals.

Unfortunately most of the first examples of such materials, such as the well-known tetrathiafulvalene-tetracyanoquindimethane,[4] present a metal-insulator transition at low temperature, due to the Peierls instability.[5,6,2] The system resembles a one-dimensional conductor spatially modulated at the Fermi wavelength in order to decrease the total energy of the electron gas. Owing to this extra modulation, the effective potential seen by each electron along the chain is quasiperiodic.

If we increase the rigidity of the material, which has been recently realized with tetramethyltetraselenafulvalane PF_6 (Ref. 7), the Peierls instability can be avoided, and leads to a conductor-superconductor phase transition, with precursor effects up to 40 K. In this paper we exhibit a simple one-dimensional model with a quasiperiodic potential for which a metal-insulator transition, as referred to above, is observed.

The investigation of the properties of the spectrum of a Hamiltonian with quasiperiodic potential is an old problem, but recently several authors[6,8–21] gave a new insight on it. Although it is known that at high energy most of the spectrum corresponds to an absolutely continuous spectral measure,[15,17] it has been conjectured that a pure point spectrum is allowed at low energy leading to a metal-insulator transition.[22]

One result in this direction has been obtained by Aubry and André[8,9] on a one-dimensional lattice model, which can be viewed as a good approximation of the Hamiltonian describing an electron of a crystal in a high magnetic field.[1,2,13,23,24]

Before the description of the model and results, we should recall some of the results of Ref. 9, where the authors consider the Hamiltonian operator acting on $l^2(Z)$ by

$$H(\lambda,\alpha,\theta)\psi(n)=\tfrac{1}{2}[\psi(n+1)+\psi(n-1)] + \lambda\cos 2\pi(\alpha-n\theta)\psi(n)\ , \qquad (1)$$

where λ is a coupling constant, α is a "random phase," and $0<\theta<1$ is an irrational number. It is simple to prove that the spectrum is independent of α but depends on (λ,θ).

Most authors were interested in the case $\lambda=1$, which corresponds to a Bloch electron in a magnetic field proportional to $1/\theta$ in connection with the de Haas–van Alphen effect. In Ref. 13 Ya Azbel proposed to relate the structure of the spectrum to the continued fraction expansion of θ.

In Ref. 24, Hofstadter computed numerically the spectrum of $H(\lambda,\alpha,\theta)$ at $\lambda=1$ as a function of θ and found a result partially in agreement with the prediction of Azbel. More recently, Aubry and André[9] gave new light on the subject studying the dependence in the coupling constant λ.

For irrational numbers θ with good diophantine approximation property, they gave convincing argument that the spectrum is absolutely continuous if $\lambda<1$ and pure point if $\lambda>1$, so the system becomes an insulator in this case. The main tool of their proof is a duality between λ and $1/\lambda$: z belongs to the spectrum of $H(\lambda,\alpha,\theta)$ if and only if $(1/\lambda)z$ belongs to the spectrum of $H(1/\lambda,\alpha,\theta)$.

More precisely, for almost every energy z there is an uniform convergence, with respect to α, of the Liapunov coefficient to the Thouless expression,[25] as in Ref. 9. From this we conclude, using the above duality, that the Liapunov coefficient is bounded below by $\ln\lambda$ and then, using an argument of Pastur[26] (see also Ref. 27), it turns out that the absolutely continuous spectrum of $H(\lambda,\alpha,\theta)$ is empty for $\lambda>1$.

On the other hand, for θ satisfying a diophantine condition, i.e.,

$$\exists\epsilon>0$$

such that

$$|n\theta-p|\geq\frac{c(\epsilon)}{n^{1+\epsilon}}\quad\forall n\in N$$

from the results of Dinaburg and Sinai[17] with duality again, we can show[16] the existence of λ_0 such that if $\lambda>\lambda_0$, the pure point spectrum of $H(\lambda,\alpha,\theta)$ is not empty, the corresponding eigenfunctions having exponential decrease and if $\lambda<1/\lambda_0$, the absolute continuum spectrum is not empty.

However, as is shown by Gordon,[19] in the case of an irrational number θ which does not fulfill the above diophantine condition, there is no eigenfunction and therefore the spectrum is singular continuous (see Ref. 10). Using computer analysis, Aubry and André found a spectrum that is a Cantor set for any values of λ with a Lebesgue measure equal to $2|1-\lambda|$. For small values of λ, the energy gaps are localized around the values of $z=\cos\pi l\theta$, $l=1,2,\ldots$ of the energy, and the widest forbidden zones correspond to the smallest values of l.

The aim of this article is to propose another kind of model which also presents a metal-insulator transition and to give a series of results, which allow us to compare the behavior of this model with the above results. Let $\hat{H}(g,\alpha,\theta)$ be the self-adjoint Hamiltonian, densely defined on $L^2(R)$ by

$$\hat{H}(g,\alpha,\theta)=-\frac{1}{2}\frac{d^2}{ds^2}-\sum_{n=-\infty}^{+\infty}g\cos2\pi(\alpha-n\theta)\times\delta(s-n)\,, \tag{2}$$

where α and θ are as in (1) and g is a coupling constant. As before, it is simple to see that the spectrum is independent of α and bounded below. This Hamiltonian differs from the one of a Krönig-Penny model[28] in that the amplitude on points $s=n$ $(n\in Z)$ is modulated in a quasiperiodic way.

A generalized eigenstate Ψ of (2) is a solution of the equation

$$\hat{H}(g,\alpha,\theta)\Psi=E\Psi\,. \tag{3}$$

If $n-1<s<n$, this equation leads to

$$\Psi(s)=A_ne^{i\sqrt{E}s}+B_ne^{-i\sqrt{E}s}\,, \tag{4}$$

with the following boundary conditions:

$$\lim_{\epsilon\to0}\Psi(n+\epsilon)-\Psi(n-\epsilon)=0 \tag{5a}$$

and

$$\lim_{\epsilon\to0}\Psi'(n+\epsilon)-\Psi'(n-\epsilon)=2g\cos2\pi(\alpha-n\theta)\Psi(n)\,. \tag{5b}$$

Inserting (5a) and (5b) into (4), we get a recursion formula of the form

$$C_{n+1}=L(\alpha-n\theta,g,\sqrt{E}\,)C_n\,, \tag{6}$$

where C_n is the column matrix

$$\begin{bmatrix}A_n\\B_n\end{bmatrix},$$

and $L(\alpha,g,\sqrt{E}\,)$ is some explicit 2×2 matrix depending on α, g, and $\sqrt{E}$.

The following change of variable simplifies (6):

$$D_n=\begin{bmatrix}1 & 1\\ e^{-i\sqrt{E}n} & e^{i\sqrt{E}}\end{bmatrix}\begin{bmatrix}e^{i\sqrt{E}n} & 0\\ 0 & e^{-i\sqrt{E}n}\end{bmatrix}C_n\,. \tag{7}$$

Now, (6) together with (7) gives the following recursion formula for the D_n, and thus for the constants A_n,B_n,

$$D_{n+1}=\begin{bmatrix} 2\cos\sqrt{E}+2g\dfrac{\sin\sqrt{E}}{\sqrt{E}}\cos 2\pi(\alpha-n\theta) & -1 \\ 1 & 0 \end{bmatrix} D_n \, . \tag{8}$$

At this stage we recognize the recursion relation of the model given by (1), namely,

$$H(\lambda,\alpha,\theta)\psi(n)=z\psi(n)\,, \tag{9}$$

with

$$D_n=\begin{bmatrix} \psi(n) \\ \psi(n-1) \end{bmatrix}, \tag{10}$$

where (z,λ) is related to (E,g) by

$$z=\cos\sqrt{E} \tag{11a}$$

and

$$\lambda=g\frac{\sin\sqrt{E}}{\sqrt{E}}\, . \tag{11b}$$

It is a matter of simple calculation to verify that the asymptotic behavior for $n\to\infty$ of D_n and C_n is equivalent, thus we get the same Liapounov exponent as well as the same rotation number for both models. Other properties of the spectra are related through the nonlinear relations (11a) and (11b). In particular, for each value of g, the set $S(\theta)$ of points (z,λ) obtained when E takes all possible values in $(-\infty,+\infty)$ resembles a snail shell (see Figs. 1 and 2) that intersects the set $\Sigma(\theta)$ of points (z,λ) for which z is in the spectrum of $H(\lambda,\alpha,\theta)$. The upper bound of the set $\Sigma(\theta)$ is given by the function

$$F(\lambda,\theta)=\|H(\lambda,\alpha,\theta)\|\, . \tag{12}$$

It follows by the Aubry-André duality that

$$F(\lambda,\theta)=\lambda F(1/\lambda,\theta)=F(-\lambda,\theta)$$

$$=F(\lambda,1-\theta)\, . \tag{13}$$

Furthermore, by a perturbative argument, we get

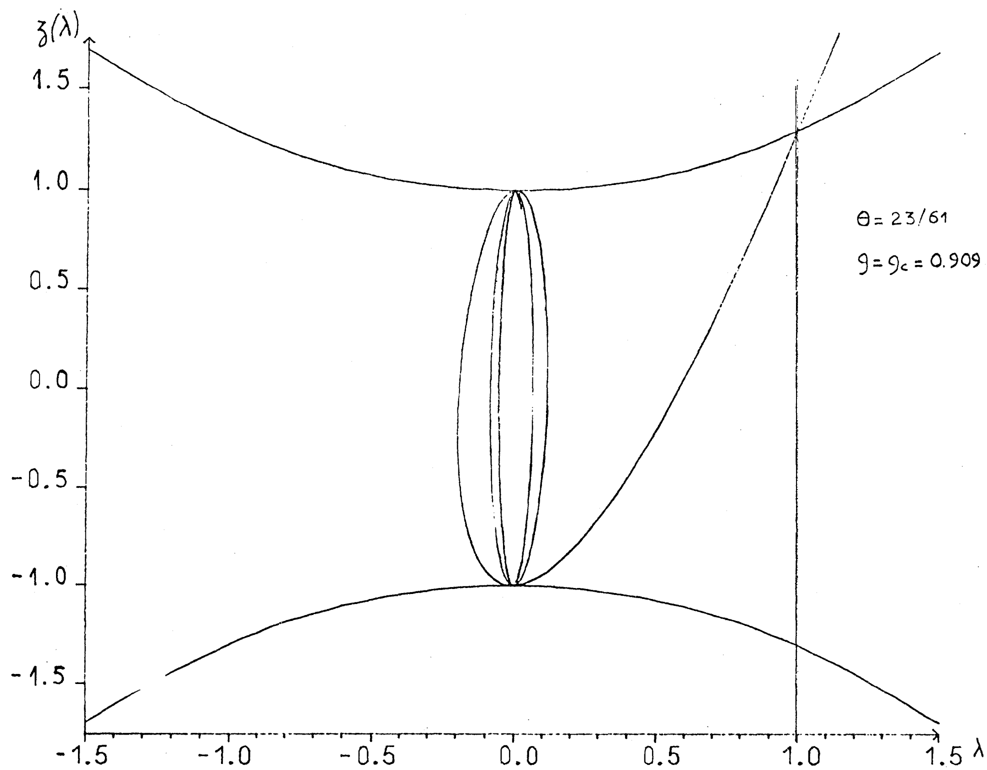

FIG. 1. For $\theta=23/61$, the representation of the "snail shell" $S(\theta)$ for $g=0.909\simeq g_c$ together with the upper and lower bounds of the spectrum.

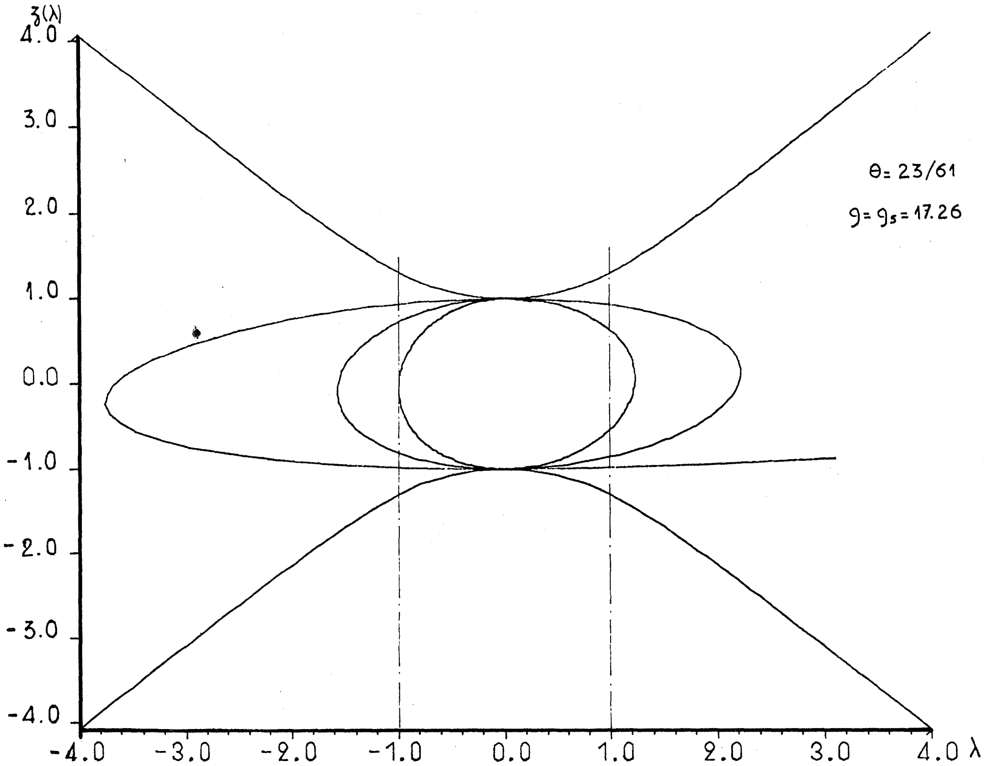

FIG. 2. For $\theta=23/61$, the representation of the "snail shell" $S(\theta)$ for $g=17.26\simeq g_5$ together with the upper and lower bounds of the spectrum.

$$F(\lambda,\theta)=1+\frac{\lambda^2}{4\sin^2\pi\theta}+O(\lambda^4) \text{ as } \lambda\to 0 , \tag{14}$$

and by (13) we also get

$$F(\lambda,\theta)=\lambda+\frac{1}{4\lambda\sin^2\pi\theta}+O(1/\lambda^3) \text{ as } \lambda\to\infty . \tag{15}$$

A closer inspection of the properties of this function[16] gives the following.

Lemma: F is a continuous function of (λ,θ) and increasing and convex function of λ for $\lambda\geq 0$.

The proof combines (12) with an approximation by Hamiltonians reduced to finite boxes. Since for $|\lambda|>1$ the spectral measure of $H(\lambda,\alpha,\theta)$ is pure point, the spectral measure of $\hat{H}(g,\alpha,\theta)$ will also be pure point in the domain of energy for which the corresponding points of $S(\theta)$ belong to $\Sigma(\theta)\cap\{(z,\lambda),\ |\lambda|>1\}$. The conditions under which such a "mobility edge" is allowed must now be determined.

The smallest value g_c of g for which this situation occurs is given by the equation

$$g_c\frac{\sin\sqrt{E_c}}{\sqrt{E_c}}=1 , \tag{16}$$

where E_c is determined by

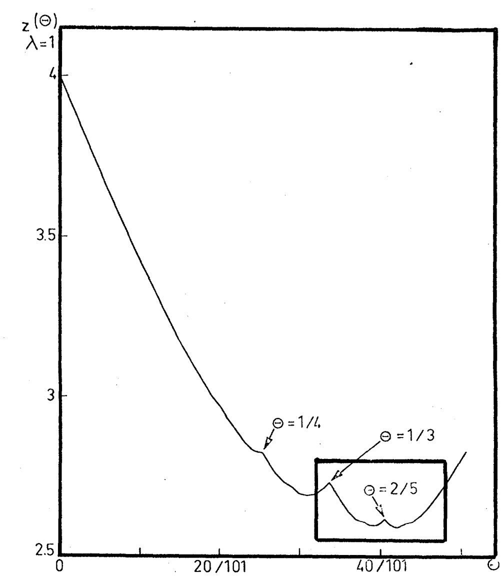

FIG. 3. The upper bound of the spectrum for $\lambda=1$.

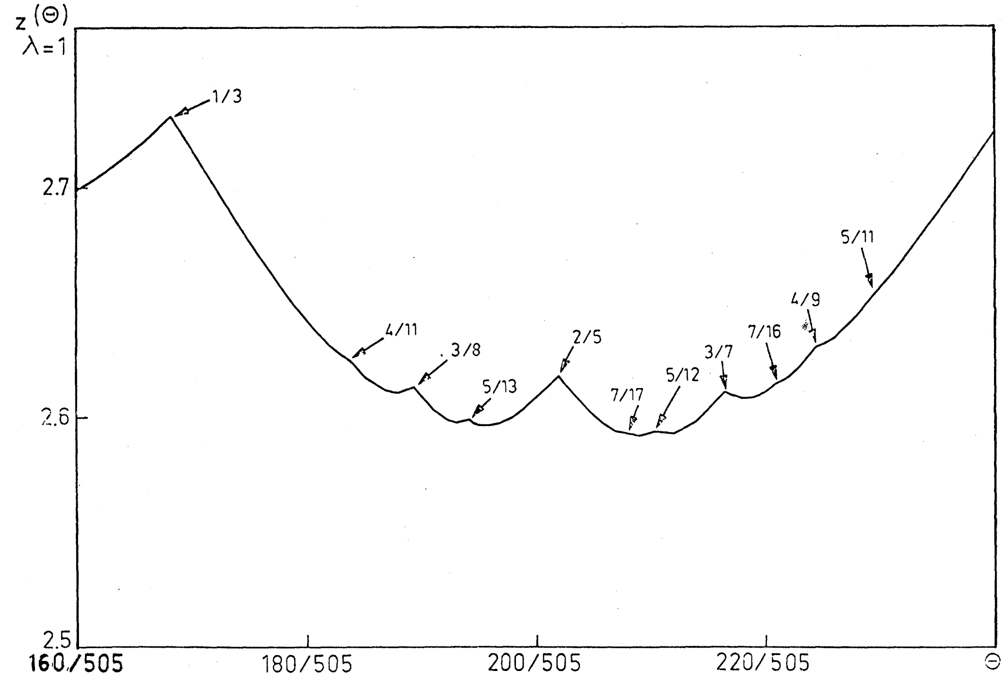

FIG. 4. Rescale of part of the curve $z(\theta)$.

$$\cos\sqrt{E_c}=F(1,\theta)\ . \tag{17}$$

Since $F(1,\theta)\geq F(0,\theta)=1$, writing $z(\theta)=F(1,\theta)$, we get

$$g_c(\theta)=\frac{\ln\{z(\theta)+[z(\theta)^2-1]^{1/2}\}}{[z(\theta)^2-1]^{1/2}}\ , \tag{18}$$

for which the following inequality is easily verified:

$$\inf_\theta g_c(\theta)\geq\frac{1}{\sqrt{3}}\ln(2+\sqrt{3})\ . \tag{19}$$

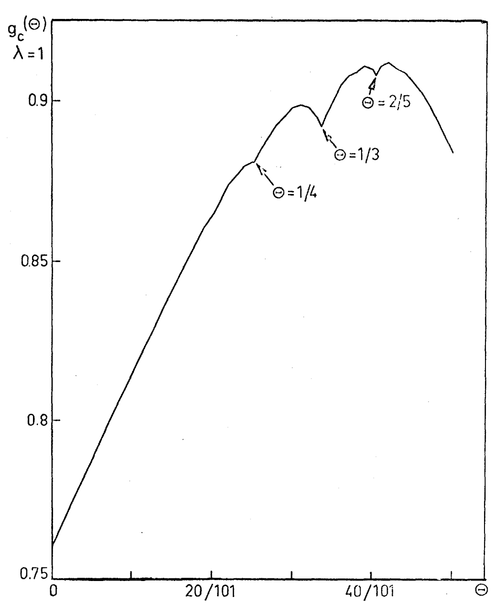

FIG. 5. Critical value of the coupling constant, function of θ.

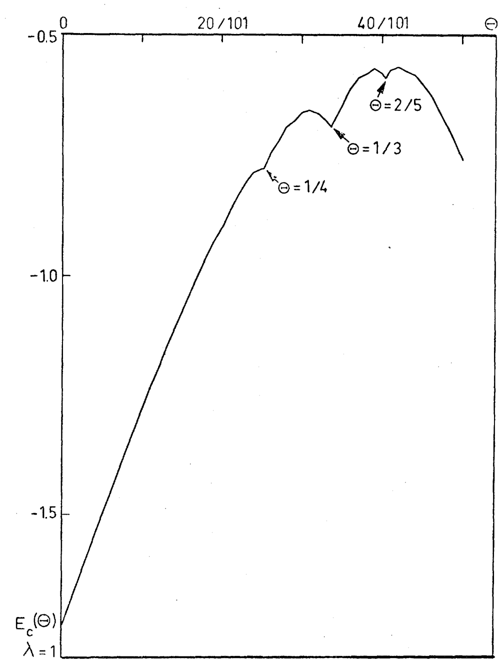

FIG. 6. Critical value of the energy as a function of θ.

An interesting feature of the model is that g_c depends in a crucial way on θ; see Fig 5. The graphs of the functions $\theta \to z(\theta)$, $\theta \to g_c(\theta)$, and $\theta \to E_c(\theta)$ are given in Figs. 3–6, using numerical computation. (Note that the first one already appears in Ref. 24.) From these figures, the curves appear to be very singular, since their derivatives seem to be discontinuous at each rational θ. Following Ref. 24, the curve $z(\theta)$ has also very interesting scaling properties. If $g < g_c(\theta)$, the spectral measure is absolutely continuous. For $g > g_c$, Figs. 1 and 2 show that the structure of the spectrum is somewhat more involved.

There is a sequence $g_c(\theta) < g_1 < g_2 < \cdots$ defined by

$$g_n \frac{\sin\sqrt{E_n}}{\sqrt{E_n}} = 1 , \tag{20}$$

and

$$\left.\frac{dg}{dE}\right|_{E=E_n} = 0 , \tag{21}$$

such that for $g_n < g < g_{n+1}$ there is a finite number of intervals $[E_i, E_i']$, $i = 0, 1, \ldots, n$ with

$$E_0 = \inf \mathrm{Sp}\hat{H}(g,\alpha,\theta) < E_0' < E_1 < \cdots < E_i < E_i' < E_{i+1} < \cdots < E_n' < +\infty , \tag{22}$$

and the spectral measure is pure point in the domain

$$\epsilon^{(g)} = \bigcup_{c=0}^{n} [E_i, E_i'] \cap \mathrm{Sp}[\hat{H}(g,\alpha,\theta)] , \tag{23}$$

and absolutely continuous outside (however, for certain values of θ, it can happen that $[E_n, E_n'] \cap \mathrm{Sp}\hat{H}(g,\alpha,\theta)$ is empty, especially if g is very close to g_n).

Combining (20) with (21) we get

$$g_n = \frac{(-1)^n}{\cos\eta_n} , \tag{24}$$

with

$$\eta_n = \tan\eta_n , \quad (2n-1)\frac{\pi}{2} < \eta_n < (2n+1)\frac{\pi}{2} . \tag{25}$$

From this we get the following values of g for the first five values of n:

$g_1 = 4.6031$,

$g_2 = 7.7926$,

$g_3 = 10.9473$,

$g_4 = 14.1029$,

$g_5 = 17.2631$.

For $n \to \infty$ the following asymptotic expression arises:

$$g_n = (2n+1)\frac{\pi}{2} - \frac{1}{(2n+1)\pi} + O(n^{-3}) . \tag{26}$$

In particular, at high energy, as is the case for regular potentials,[17] the spectrum is a Cantor set of positive Lebesgue measure and the spectral measure is absolutely continuous; see also Refs. 15 and 16.

Note added. A similar change of variables allows us to have the same kind of informations on the spectrum of a more general Kronig-Penny model, namely,

$$H(f,g,\alpha,\theta) = -\frac{1}{2}\frac{d^2}{ds^2} - \sum_{n\in Z} g \cos 2\pi(\alpha - n\theta) \times \delta(s - s_n) , \tag{27}$$

where $f = \{f_n\}_{n\in Z}$ is an almost periodic sequence, with $f_n \geq a > 0$, which fixes the points s_n by $s_n - s_{n-1} = f_n$. Changing variables as in (7), but with s_n replacing n, easily gives rise to the following recursion formula, which replaces (8):

$$D_{n+1} = \begin{pmatrix} \dfrac{\sin(f_n + f_{n+1})\sqrt{E}}{\sin f_n\sqrt{E}} + 2g\cos 2\pi(\alpha - n\theta)\dfrac{\sin f_{n+1}\sqrt{E}}{\sqrt{E}} & -\dfrac{\sin f_{n+1}\sqrt{E}}{\sin f_n\sqrt{E}} \\ 1 & 0 \end{pmatrix} D_n . \tag{28}$$

This formula corresponds to a (gauge) modified Aubry model. Other generalizations can be derived in the same way and we plan to discuss these cases in a forthcoming paper.[16]

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